Part 11: Genetic Algorithms

February 8, 2021

Hope everyone had a great weekend! I don't think I mentioned last week what we were going to talk about but based on the title its Genetic Algorithms (GA). A GA is a derivative free optimization method (sometimes called zeroth order) that is quite popular for its ease of implementation.

1 Basics of Genetic Algorithms

Okay to start off, a GA is an iterative method that changes some parameters X to optimize an output Y. It has four distinct parts: (i) Selection, (ii), Crossover, (iii) Combination, and (iv) Mutation. We will use the following toy function as an example:

$$f(x) = x_1^2 - 0.5x_1 + 1 + U(-0.2, 0.2)$$

1.1 Selection

Let's say you have some initial data $\{X, Y\}$ where $Y = f(X)$. Start by ranking X from best to worst based on the output Y. We'll do this in a *Roulette Wheel* method where the probability of picking a point x from X is proportional to the quality metric Y. From a database of $N = 10$ we'll select $N/2$ points.

1.2 Crossover and Combination

Next we crossover the best points by randomly choosing two points of the $N/2$ selected points and creating a new point x_{child} from a random selection of those points x_{parent}. In our code we generate a "cut point" c where one parent gives their input data to the left of c, and the other parent gives their input data to the right c.

$$x_{child} = x_{parent,1}[:c] \cup x_{parent,2}[c:]$$

We then combine the $N/2 = 5$ parents and their $N/2 = 5$ children to get the next generation.

$$X = X_{parent} \cup X_{children}$$

1.3 Mutation

The final stage is mutation, where we introduce random perturbations to this next generation of X points. Mutation allows the algorithm to not get stuck in local optima. There are many methods, but we will simply randomly resample all i points and j parameters x_{ij} with some probability p_{mut} in the bounds B of the point/parameter pair. In our example problem, with $N = 10$ for 10-dimensional problem, we set $p_{mut} = 10^{-2}$. Therefore, an average of $100 * 10^{-2} = 1$ mutations will occur per iteration of the GA.

The whole algorithm is shown below in Algorithm 1.

We run $M = 2000$ GA simulations over $f(x)$ where minimization is the goal which is shown in Figure 1.

2 Solving A Multi-Fidelity GP Model with GAs

We now move on from the toy model to a harder one, maximizing the likelihood of a multi-fidelity gaussian process model (GP). You don't need to know why, but the likelihood of a multi-fidelity GP model for given hyperparamters θ will be as follows:

$$log(L) = -0.5log(det(K_y)) - 0.5Y^T(K_y)^{-1}Y - N/2log(2\pi) - 0.5(\theta - \bar{\theta})^T\Sigma^{-1}(\theta - \bar{\theta})$$

$$k_y = K(X, X) + \sigma_n^2$$

Which differs slightly from our usual $L(\theta)$ equation from Post 2 via the $-0.5(\theta - \bar{\theta})^T\Sigma^{-1}(\theta - \bar{\theta})$ term. This term represents a prior normal distribution (or rather

Initialize X, Y, K ;
for $k = 1 : K$ **do**
  for *Selection* **do**
    $p \propto Y$;
    $X_{keep} \longleftarrow X$;
  end
  for *Crossover* **do**
    for $i = 1 : N/2$ **do**
      $x_{child,i} = x_{parent,1}[: c] \cup x_{parent,2}[c :]$
    end
  end
  for *Combination* **do**
    $X = X_{parent} \cup X_{children}$
  end
  for *Mutation* **do**
    $Pr(x_{i,j} = U(B_{ij})) = p_{mut}$
  end
end

Algorithm 1: Genetic Algorithm

the log of that distribution) for the hyperparameters. The model itself looks very much like the GP we used previously:

$$\mu(x^*) = K(x^*, X)^T (K_y)^{-1} Y$$

$$\sigma^2(x) = k(x^*, x^*) - K(x^*, X)(K_y)^{-1} k(x^*, X)^T$$

The major difference is the kernel matrix $K(x, x')$ which is as follows:

$$K(x, x') = K_0(x, x') + \{IS \neq 0, IS = IS'\} K_l(x, x')$$

Where $K_0(x, x')$ is a squared exponential kernel for regression over a 'primary' information source (a really good model for example) and $K_l(x, x')$ is the kernel for data from l information source (a less good model for example). We will solve the problem $\theta^* = argmin - log(L(\theta))$ for a given set of data of $|l| = 3$ sources of information using the GA developed above. We will be going into how this work

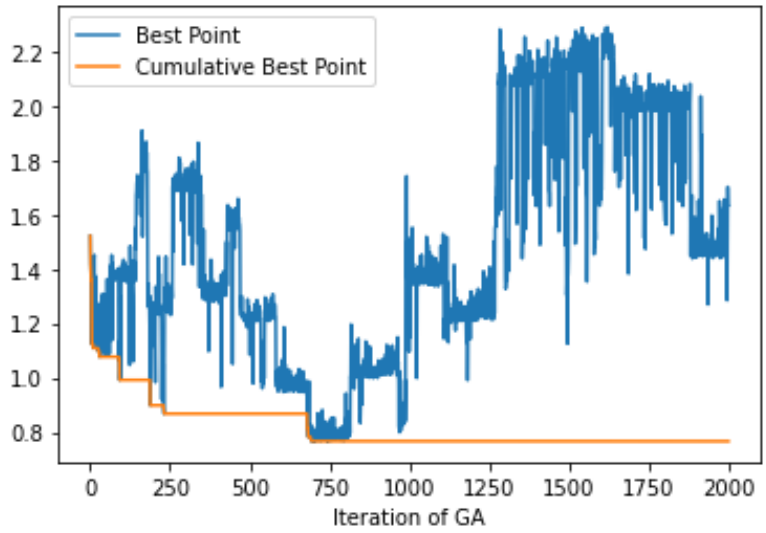
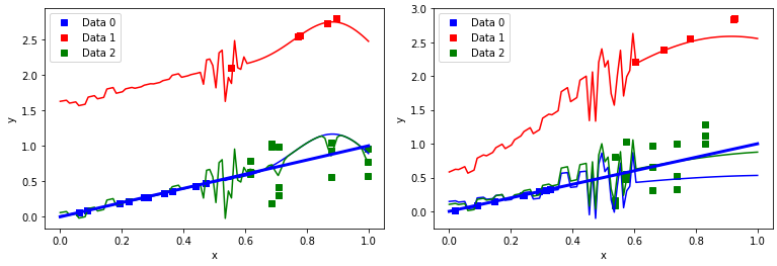


Figure 1: GA Solving $f(x)$ | $p_{mut} = 0.01$, $N = 10$, $M = 2000$

in future posts (because it is also a big part of a new project I am working on) but suffice to say it'll be interesting. Here is the result using l-BFGS-B optimizer which approximates its own Hessians and gradients versus the same model for a GA.



(a) L-BFGS-B (b) GA

Figure 2: Multi-Fidelity GP

Also noting the convergence results of the GP.

I actually didn't realize until I was running the GA that **it takes forever**. Note from Figure 3 we are using $N = 10$ per round of $M = 100$ generations. This means $M * N$ calculations need to be made with the matrix inverse to calculate $-log(L(\theta))$. Funny enough, the best solution was found almost immediately and

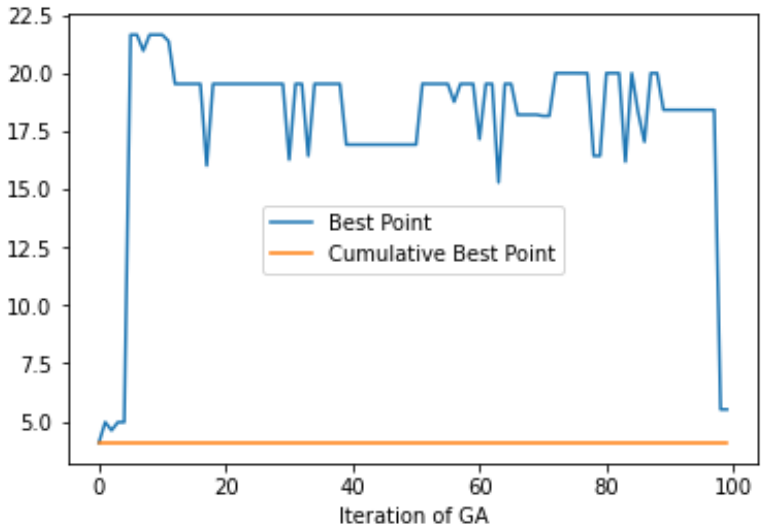


Figure 3: GA Solving Multi-Fidelity GP | $p_{mut} = 0.01$, $N = 10$, $M = 100$

doesn't look too different from the L-BFGS-B solution (note to self, change bounds of GA to be in line with L-BFGS-B haha). This proves an important point, that GAs are very useful for cheaply solved functions like the toy function from Part 1, but not for expensive ones. This actually is a big theme in optimization, that problem complexity may determine which method you can use.

Well that's all folks. This time I'll tell you what we'll be working on next week. It'll be a continuation of this work on the multi-fidelity GPs!